A computational approach to predicting the structure of nano-alloy catalysts revealed

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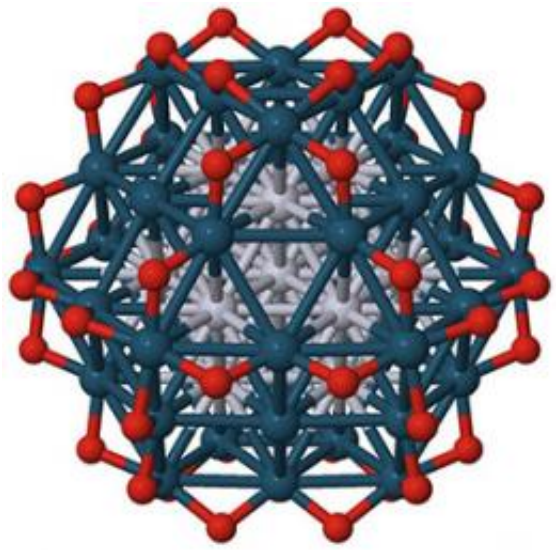

Calculations show that platinum-core (gray)–palladium-shell (green) nanoparticles are particularly stable. Hydrogen atoms (red) that adsorb to the particle surface are catalytically converted into hydrogen gas. Credit: 2012 A*STAR Institute of High Performance Computing

Nanoparticles can be potent catalysts. Bimetallic nano-alloys of platinum and palladium, for example, can help to generate hydrogen fuel by promoting the electrochemical breakdown of water. Identifying the most active nano-alloy for such a task, however, remains a challenge; catalytic performance relates directly to particle structure, and experiments to establish the atomic arrangement of such small particles are difficult to perform. Predicting stable nano-alloy structures is now possible using a

computational approach developed by Teck Leong Tan at the A*STAR Institute of High Performance Computing and his co-workers. Their technique can also identify ways in which the nanoparticle's atomic structure could be tuned to improve catalytic performance.

The challenge with calculating nano-alloy structure and properties from first principles is the computational processing power it requires, says Tan. For their study, he and his co-workers considered a 55-atom nano-alloy particle, each site in the structure filled by either a palladium or a platinum atom. "There are millions of possible alloy configurations, so it would be computationally intractable to do a direct search using first-principles calculations," Tan explains.

To make the process manageable, the researchers conceptually broke the nanoparticle down into small geometric subunits, or clusters. From first principle calculations on a set of around 100 different alloy structures, each consisting of 30 or so clusters, they generated a reliable model of alloy behavior using an approach called cluster expansion. From this model, they calculated whole-nanoparticle properties. "The model is used to rapidly search through the huge configuration space for low-energy states," says Tan. These low-energy states represent the stable alloy configurations that should exist experimentally (see image).

Using their calculated stable structures, Tan and his co-workers then predicted how different atomic conformations affect a particle's performance as a catalyst. As a model reaction, the researchers examined the hydrogen evolution reaction, the electrochemical generation of hydrogen gas. The results suggest that particle catalytic activity will increase as more palladium is added, because this alloy improves hydrogen binding at various adsorption sites on the nanoparticle surface—useful information for guiding the synthesis of new nanocatalysts.

The approach should be widely applicable for nanoparticle research, notes Tan. "The cluster expansion method can generally be applied to any alloy systems where structures and stabilities are of interest," he says. Tan next plans to investigate the impact of molecules adsorbed onto a catalyst's surface. "The presence of adsorbed molecules often leads to changes in alloy structures, thereby altering catalytic performance," he says.

More information: Tan, T. L., Wang, L. -L., Johnson, D. D. & Bai, K. A comprehensive search for stable Pt–Pd nanoalloy configurations and their use as tunable catalysts. *Nano Letters* 12, 4875–4880 (2012). pubs.acs.org/doi/abs/10.1021/nl302405k

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